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Surface-roughness fractality effects in electrical conductivity of single metallic and semiconducting films

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Surface-roughness effects in electrical conductivity of thin metallic and semiconducting films with self-affine fractal surfaces are considered in the framework of the Born approximation. The surface roughness is described by the k-correlation model, and is characterized by the roughness exponent H $(0 \leqslant H \leqslant 1)$, the in-plane correlation length ξ, and the rms roughness amplitude Δ. In the case of metallic films the conductivity is shown to increase monotonically with H increasing from $H=0$ to $H=1$ and with decreasing ratio Δ/ξ. For semiconducting quantum wells the conductivity shows a peculiar interplay of quantum-mechanical effects and scattering due to surface roughness. [S0163-1829(97)02431-4]

I. INTRODUCTION

Early experiments on electronic transport in metallic thin films clearly showed the existence of substantial electron scattering by roughness of the film surfaces.[1] The problem of surface influence on electrical conductivity of thin metallic films has been known for a long time, and was first encountered by Thompson[2] at the beginning of this century. It was considered later in more detail by Fuchs,[3] who formulated the first quasiclassical theory of the size effects (so-called classical size effect). In the framework of this theory, electron scattering on rough surfaces is included by some phenomenological parameters which enter boundary conditions imposed on the electron distribution function. Further development of the theory of classical size effects resulted in a transformation of the Fuchs boundary conditions into more realistic integral-type boundary conditions.[4]

Owing to the recent progress in the technology of controlled fabrication of quasi-two-dimensional thin films, recent experiments on the conductivity of metallic[5,6] and semiconducting[7] films revealed features of the transport properties and gave clear evidence of some deviations from the quasiclassical theory. The first quantum-mechanical description of the film conductivity was developed by Prange and Nee,[8] and applied to semiconducting thin films,[7] where the molecular-beam-epitaxy (MBE) technique allows one to construct quantum wells which are thinner than 10 nm. Later treatments were based on the Green-function formulations[9] and coupled Boltzmann-like equations.[10–12]

The approach of Fishman and Calecki[11] was applied to account for the universal power law, $\sigma \propto d^c$ (with $c \approx 2.3$), in the variation of the film conductivity σ with increasing film thickness d, which was observed in very thin $CoSi_2$ films grown by MBE.[5] A similar law, but with $c \approx 6$, was also found in the case of semiconducting thin films. Apart from this, Fishman and Calecki[12] showed that the form of the height-height correlation function plays a significant role in the limit $k_F \xi \gg 1$, where k_F is the Fermi wave vector and ξ is the in-plane correlation length for the surface roughness. Moreover, they showed that for $k_F \xi \gg 1$ the mean variation of σ with the film thickness d cannot be approximated by the power laws described above. Analytical results were obtained for two forms of the correlation function, i.e., for the exponential, $\propto \exp[-(r/\xi)]$, and Gaussian, $\propto \exp[-(r/\xi)^2]$, forms.

In this paper we generalize a description of the influence of the form of the correlation function on the film conductivity to surfaces with self-affine and logarithmic roughness. The roughness will be described in terms of an analytic correlation model in Fourier space,[13] which interpolates between correct asymptotics that characterize those categories of surfaces. The self-affine fractal surface/interface roughness is characterized, in addition to the root-mean-square deviation Δ from flatness and the average distance between consecutive peaks or valleys attributed to the correlation length ξ, also by a local fractal dimension d_f $(d_f = 3 - H$, where H is the roughness exponent, $0 \leqslant H \leqslant 1)$ that characterizes the degree of surface irregularity. The approach is valid for correlation lengths longer than the interatomic distance.

The paper is organized as follows. In Sec. II we present a theoretical description of the film conductivity in the case where the confining potential is infinite, and surface roughness is the only source of diffuse electron scattering. The self-affine fractal model of the film surfaces is described in Sec. III. Special cases where some analytical results can be obtained for the matrix describing interminiband and intraminiband transition probabilities are discussed in Sec. IV. Results for electrical conductivity in semiconducting and metallic films are described respectively in Secs. V and VI. A general case, with finite confining potential and bulk impurity scattering, is presented in Sec. VII. Finally, some general conclusions are presented in Sec. VIII.

II. THIN-FILM CONDUCTIVITY

The following description of the thin-film conductivity is based on the theory developed by Fishman and Calecki.[11,12] Assume as in Ref. 11 that the bottom and top boundaries of a conducting film are defined by the equations $z=-d/2$ and $z=d/2+h(\mathbf{r})$, respectively. For simplicity, we assume here that only the upper surface of the film is rough, with the roughness described by a single-valued random function $h(\mathbf{r})$ of the in-plane position vector $\mathbf{r}=(x,y)$. Moreover, the roughness is assumed to be isotropic, such that the height-height correlation function $C(r)=\langle h(\mathbf{r}')h(\mathbf{r}'')\rangle$ depends only on the relative distance $r=|\mathbf{r}'-\mathbf{r}''|$.

Assuming that only the surface roughness contributes to electron scattering, one finds, in the Born approximation, the following expression for the film conductivity:[11]

$$\sigma=\frac{e^2\hbar^3}{m^2d}\sum_{\nu=1}^{N}\sum_{\nu'=1}^{N}k_\nu^2k_{\nu'}^2[C^{-1}]_{\nu\nu'}, \tag{1}$$

where m is the electron mass, N denotes the number of occupied minibands, and $k_\nu=[(2m/\hbar^2)(E_F-E_\nu)]^{1/2}$, with E_F and E_ν being, respectively, the Fermi energy and the energy minimum of the νth miniband (miniband edge). In Eq. (1) $C_{\nu\nu'}$ is a matrix which is determined by interminiband and intraminiband transitions due to electron scattering, and which for infinite confining potential assumed here is of the form

$$C_{\nu\nu'}=\delta_{\nu\nu'}A_\nu k_\nu^2\sum_{\mu=1}^{N}A_\mu(F_1)_{\mu\nu}-A_\nu A_{\nu'}k_\nu k_{\nu'}(F_2)_{\nu\nu'}, \tag{2}$$

where $A_\nu=\hbar^2\pi^2\nu^2/md^3$, and

$$(F_1)_{\mu\nu}=\int_0^{2\pi}\langle|h(k_{\mu\nu})|^2\rangle d\theta,$$

$$(F_2)_{\nu\nu'}=\int_0^{2\pi}\langle|h(k_{\nu\nu'})|^2\rangle\cos\theta\, d\theta, \tag{3}$$

with $\langle|h(k)|^2\rangle$ the Fourier transform of the height-height correlation function $C(r)$, and

$$k_{\nu\nu'}=(k_\nu^2+k_{\nu'}^2-2k_\nu k_{\nu'}\cos\theta)^{1/2}. \tag{4}$$

The Fermi energy E_F for a particular film thickness d and a given carrier density n is determined by the condition

$$nd=\frac{m}{\pi\hbar^2}\sum_{\nu(E_\nu<E_F)}\int_{-\infty}^{E_F}\Theta(E-E_\nu)dE, \tag{5}$$

where $\Theta(x<0)=0$ and $\Theta(x\geq 0)=1$ by definition. After integrating over the energy E, this condition acquires the form

$$nd=\frac{m}{\pi\hbar^2}\left\{NE_F-\sum_{\nu=1}^{N}E_\nu\right\}. \tag{6}$$

Taking into account the fact that for infinite confining potential the discrete energy levels E_ν (miniband edges) are given by the formula $E_\nu=(\hbar^2/2m)(\nu\pi/d)^2$, one can easily determine from Eq. (6) both the Fermi energy E_F and the number N of occupied minibands.

III. SELF-AFFINE FRACTAL MODEL

The correlation function for any physical self-affine surface is characterized by a finite correlation length ξ, which is a measure of the average distance between peaks and valleys on the surface such that $C(r)\approx\Delta^2-Dr^{2H}$ for $r\ll\xi$ and $C(r)=0$ for $r\gg\xi$ ($D\sim\Delta^2/\xi^{2H}$ is a constant).[13–16] The roughness exponent $0\leq H\leq 1$ is a measure of the degree of surface irregularity.[14,16] Small values of H characterize jagged or irregular surfaces at short length scales ($r\ll\xi$), where the correlation function shows power-law behavior, while large values of H correspond to smoother height-height fluctuations. For example, see Fig. 1 in Ref. 17, where the self-affine curves for $H=0.3$, 0.5, and 0.7 are plotted with the same rms width $\Delta=1.1\pm0.1$ to show the effect of the roughness exponent H. Similar plots can also be found in Ref. 18.

For self-affine fractals the Fourier transform $\langle|h(k)|^2\rangle$ of $C(r)$ has the scaling behavior $\langle|h(k)|^2\rangle\propto k^{-2-2H}$ if $k\xi\gg1$, and $\langle|h(k)|^2\rangle\propto$const if $k\xi\ll1$.[13] The self-affine scaling behavior in the asymptotic limits $k\xi\gg1$ and $k\xi\ll1$ is satisfied by the k-correlation model,

$$\langle|h(k)|^2\rangle=(2\pi)\frac{\Delta^2\xi^2}{(1+ak^2\xi^2)^{1+H}}. \tag{7}$$

In the intermediate length scales, Eq. (7) is an approximation which, however, gives results in agreement with experiments.[13,15] The normalization condition $\int_{0<k<k_c}\langle|h(k)|^2\rangle d^2\mathbf{k}=(2\pi)^2\Delta^2$ yields the parameter a in the form $a=(1/2H)[1-(1+ak_c^2\xi^2)^{-H}]$ for $0<H\leq1$, and $a=(1/2)\ln(1+ak_c^2\xi^2)$ for $H=0$. Here, $k_c=\pi/a_0$ is the upper cutoff in the Fourier space, with a_0 denoting the atomic layer spacing. Expressions valid for $H=0$ can be obtained from those valid for $H>0$, if we consider the identity $\lim_{H\to0}(1/H)[x^H-1]=\ln(x)$. The limiting case of logarithmic roughness ($H=0$) is related to predictions of various growth models for the nonequilibrium analog[19] of the equilibrium roughening transition.[20] For $H=0.5$ and $k_c\xi\gg1$, Eq. (7) yields exactly the Fourier transform of the simple exponential correlation function.

IV. ANALYTICAL RESULTS FOR $(F_i)_{\mu\nu}$ ($i=1$ and 2)

For $H=0$ and 1 the integrals in Eq. (3) can be calculated exactly, and one can obtain analytical expressions for the film conductivity. For this purpose, we define the quantities

$$\Gamma_{\nu\nu'}=1+a\xi^2(k_\nu^2+k_{\nu'}^2) \tag{8}$$

and

$$B_{\nu\nu'}=2ak_\nu k_{\nu'}\xi^2/\Gamma_{\nu\nu'}. \tag{9}$$

(a) $H=0$: The case $H=0$ (logarithmic roughness) resembles correlations observed in liquids due to thermally induced capillary waves.[21] Calculations of the integrals in Eq. (3) yield

$$(F_1)_{\nu\nu'}=\frac{(2\pi\Delta\xi)^2}{(1+\Gamma_{\nu\nu'})[1-B_{\nu\nu'}^2]^{1/2}}, \tag{10}$$

$$(F_2)_{\nu\nu'}=\frac{(2\pi\Delta\xi)^2}{B_{\nu\nu'}}\left\{1-\frac{1}{(1+\Gamma_{\nu\nu'})[1-B^2_{\nu\nu'}]^{1/2}}\right\}. \tag{11}$$

(b) $H=1$: This is a peculiar case which does not represent strictly speaking a self-affine fractal structure and is rather related to the formation of large mountain-valley surface structures.[18] Calculations of the integrals in Eq. (3) now yield

$$(F_1)_{\nu\nu'}=\frac{(2\pi\Delta\xi)^2 B_{\nu\nu'}}{(1+\Gamma_{\nu\nu'})^2}\left\{\frac{1}{(1-B^2_{\nu\nu'})^{1/2}}+\frac{B_{\nu\nu'}}{(1-B^2_{\nu\nu'})^{3/2}}\right\}, \tag{12}$$

$$(F_2)_{\nu\nu'}=\frac{(2\pi\Delta\xi)^2 B_{\nu\nu'}}{(1+\Gamma_{\nu\nu'})^2}(1-B^2_{\nu\nu'})^{-3/2}. \tag{13}$$

(c) $0<H<1$: For the case $0<H<1$ (self-affine fractal roughness) we still can find some analytical results, if we expand the denominator of the integrand in the integrals of Eq. (3). Indeed, we have the expansion $[1-B_{\nu\nu'}\cos\theta]^{1+H}\approx[1-(1+H)B_{\nu\nu'}\cos\theta+\cdots]$ if and only if $|B_{\nu\nu'}|\ll 1$. Thus we obtain the following approximate expressions:

$$(F_1)_{\nu\nu'}\approx(2\pi\Delta\xi)^2(\Gamma_{\nu\nu'})^{-1-H}(1+\Gamma_{\nu\nu'})^{-1}\times[1-\{(1+H)B_{\nu\nu'}\}^2]^{-1/2}, \tag{14}$$

$$(F_2)_{\nu\nu'}\approx(2\pi\Delta\xi)^2[(1+H)B_{\nu\nu'}]^{-1}(\Gamma_{\nu\nu'})^{-1-H}\times\{1-(1+\Gamma_{\nu\nu'})^{-1}[1-\{(1+H)B_{\nu\nu'}\}^2]^{-1/2}\}. \tag{15}$$

However, caution is required in the use of these approximations, since the conditions of their validity should be satisfied for the involved surface parameters (H,ξ) and the wave vectors k_ν.

V. CONDUCTIVITY FOR SEMICONDUCTING QUANTUM WELLS

Since the areal electron concentration in semiconducting films can be rather low (e.g., in GaAs quantum wells[7] $nd\approx 3\times10^{-3}$ nm^{-2}), the number N of occupied minibands can be small too, say $N=1$ or 2. For $N=1$ one can easily derive some analytical expressions for the electrical conductivity. Indeed, for infinite confining potential one finds from Eqs. (1) and (2) the following formula for the film conductivity:

$$\sigma=G_0\left\{\frac{4n}{\pi^2}\left[\int_0^{2\pi}\langle|h(q)|^2\rangle(1-\cos\theta)d\theta\right]^{-1}\right\}d^6, \tag{16}$$

where

$$q=[4\pi nd(1-\cos\theta)]^{1/2} \tag{17}$$

and $G_0=e^2/2\pi\hbar=e^2/h$.

From Eq. (16) we directly observe the power-law behavior of the film conductivity vs film thickness, $\sigma\propto d^6$, which has been found in semiconducting films.[7] For the roughness exponents $H=0$ and 1, Eq. (16) yields the simple analytical expressions

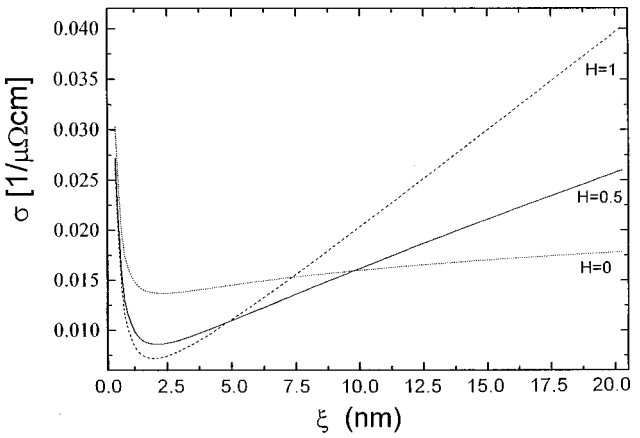

FIG. 1. Electronic conductivity σ of a quantum well ($N=1$) vs correlation length ξ for $d=5$ nm ($d<d_c$), $a_0=0.3$ nm, $\Delta=0.3$ nm, and H, as indicated.

$$\sigma=\frac{G_0 n}{\pi^4\Delta^2\xi^2}\left\{\frac{B(1+\Gamma)(1-B^2)^{1/2}}{(B-1)-(1+\Gamma)(1-B^2)^{1/2}}\right\}d^6 \tag{18}$$

for $H=0$, and

$$\sigma=\frac{G_0 n}{\pi^4\Delta^2\xi^2}\left\{\frac{(1+\Gamma)^2(1-B^2)^{3/2}}{B^2(1+B)}\right\}d^6 \tag{19}$$

for $H=1$, where $\Gamma=1+2a\xi^2k^2$, $B=2ak^2\xi^2/\Gamma$, and $k=(2\pi nd)^{1/2}$.

In Fig. 1 we present the film conductivity σ vs correlation length ξ for several values of the roughness exponent H. The numerical results were obtained from Eq. (16), and are shown for the areal electron density equal to 4×10^{-2} nm^{-2} and the film thickness $d=5$ nm. The well width d is smaller than the critical value $d_c=10$ nm, where the Fermi level crosses the bottom of the second miniband. In other words, this value of d corresponds to the case where only one electron miniband is occupied ($N=1$). The effect of the form of correlation function on the ratio of electron mobility below and above d_c was investigated in Ref. 11. In this paper, however, we limit considerations to the case $d<d_c$. A characteristic feature seen in Fig. 1 is the presence of a minimum in the film conductivity as a function of the correlation length, which occurs approximately at $\xi=2$ nm. For large values of ξ the conductivity displays a *normal* behavior, i.e., it increases with increasing H or increasing ξ (decreasing ratio Δ/ξ, surface/interface smoothing). For small values of ξ ($\xi<2$ nm) the situation is reversed, i.e., the conductivity increases with decreasing H and decreasing ξ. This is due to the fact that this kind of roughness does not scatter electrons when their wavelength is much longer than the correlation length ξ. In the intermediate range the appropriate behavior is more complex, i.e., the conductivity has a minimum in the dependence on H. This is shown more explicitly in Fig. 2, where the dependence of the film conductivity on the roughness exponent H is shown for several values of the correlation length ξ. For $\xi=2.5$ nm the conductivity decreases with increasing H, whereas for larger values of ξ ($\xi=5$, 7.5, and $\xi=12$ nm), it first decreases with increasing H, reaches a minimum, and then increases with a

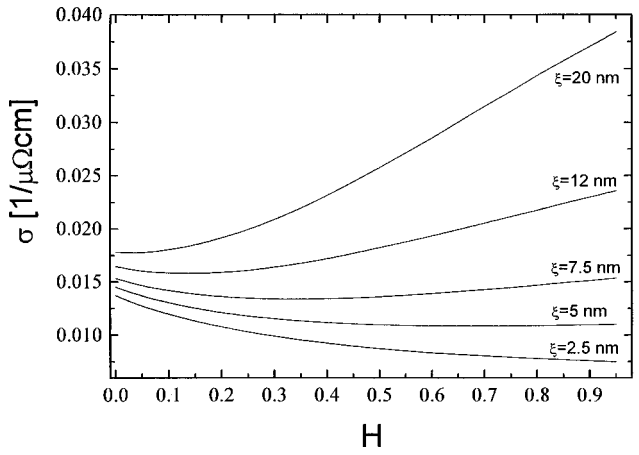

FIG. 2. Conductivity σ vs H for $d=5$ nm ($d<d_c$), $a_0=0.3$ nm, $\Delta=0.3$ nm, and ξ, as indicated.

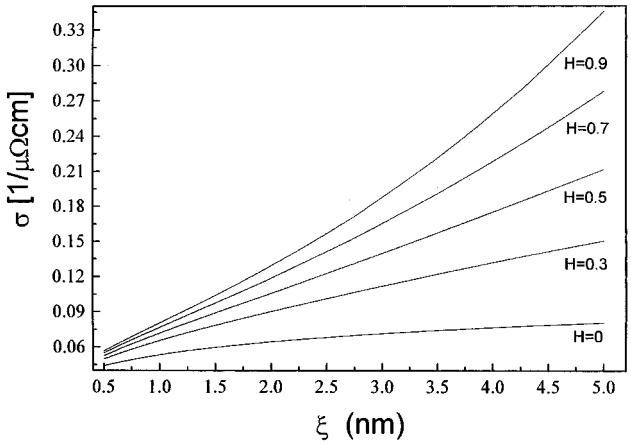

FIG. 3. Conductivity σ vs correlation length ξ for $d=2$ nm, $a_0=0.3$ nm, $\Delta=0.3$ nm, and H, as indicated.

further increase of the roughness exponent H. For $\xi=20$ nm the conductivity increases with increasing H in the whole range $0<H<1$.

VI. RESULTS FOR METALLIC FILMS

Now, we will concentrate on metallic films ($N\gg1$), and assume in our calculations parameters typical for $CoSi_2$ (bulk carrier density $n\approx3\times10^1$ nm^{-3}). The parameter Δ varies usually in a small range between one to two interatomic distances, and in the following we assume $\Delta=0.3$ nm. On the other hand, the parameter ξ for the $CoSi_2$/Si interface is also of an order of interatomic distances,[5] However, for systems with excellent surfaces the correlation length may be quite large,[22] as is indicated by mobility experiments on GaAs/AlAs interfaces[7] and high-resolution transmission electron microscopy on Si/SiO_2 interfaces.[23]

Regarding the surface/interface roughness parameters Δ, ξ, and H, we point out the following. The ratio Δ/ξ describes behavior of the surface at large length scales ($r>\xi$), where, for a large variety of growth studies, $\Delta/\xi<0.5$.[18] At small length scales ($r<\xi$) the roughness is characterized by the roughness exponent H. For thin films and for roughness parameters such that $H\sim1$ and $\Delta/\xi\ll1$, the interface scattering is weak (since the surfaces have rather smooth characteristics at all length scales), which results in a higher conductivity and more pronounced quantum-mechanical effects.

The influence of the autocorrelation function on the thickness dependence of the electrical conductivity was investigated already by Fishman and Calecki.[12] We remark that the conductivity σ increases with increasing d and increasing H, approaching the largest values for $H\sim1$. Figure 3 depicts the conductivity σ vs correlation length ξ for the film thickness $d=2$ nm (ultrathin regime) and for several values of the roughness exponent H. For the correlation lengths of the order of d or smaller, the conductivity σ shows a similar rate of increment for different values of H. However, at large ξ the conductivity increases with increasing ξ at a much faster rate for large H ($H\sim1$). On the other extreme limit, as can be seen from the curve that corresponds to the logarithmic roughness ($H=0$), the conductivity increases extremely slowly with increasing correlation length (decreasing ratio Δ/ξ). Thus the smoothing effect at large length scales is strongly influenced by the roughness exponent. Indeed, the conductivity can increase by one order of magnitude at large $\xi(d\ll\xi)$ when the roughness exponent varies from $H=0$ to $H=1$.

Figure 4 shows the conductivity σ vs roughness exponent H for $d=2$ nm and various correlation lengths. The conductivity increases rather slowly with increasing H for the correlation lengths of about the same size as the film thickness d. However, it increases much faster for $H>0.5$ and large $\xi(d<\xi)$. In the latter case the conductivity can increase by an order of magnitude as the roughness exponent H increases from 0 to 1. Thus the film conductivity for large correlation lengths (or $\Delta/\xi\ll1$) is significantly influenced by the fractality effects which can play an important role in electrical transport properties.

VII. GENERAL MODEL

The model used above includes the following simplifications: (i) It takes into account roughness of only one of the two surfaces. (ii) The confining potential is infinite on both sides of the structure. (iii) It does not take into account electron scattering on impurities and/or other structural defects

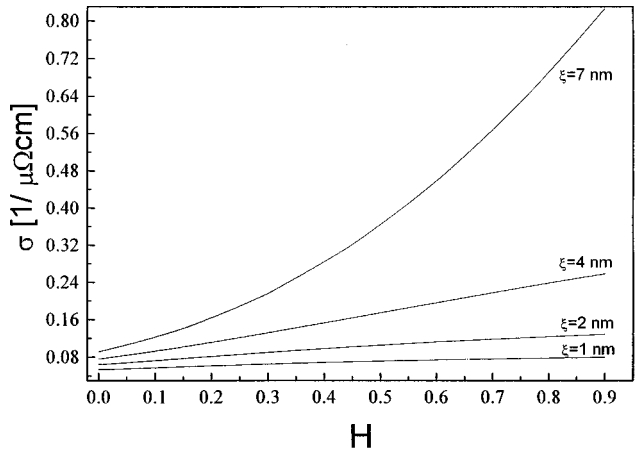

FIG. 4. Conductivity σ vs roughness exponent H for $d=2$ nm, $a_0=0.3$ nm, $\Delta=0.3$ nm, and indicated values of ξ.

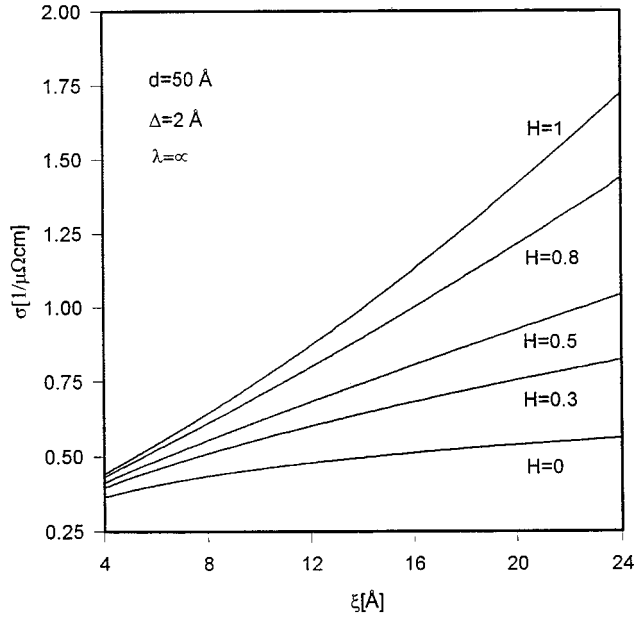

FIG. 5. Conductivity σ vs correlation length ξ for $U_{\text{conf}}=8.5$ eV, $\mu=3.5$ eV, and $a_0=0.3$ nm. The other parameters are as indicated.

distributed inside the film. In a general case the situation is more complex, and all the above factors have to be included into considerations. Moreover, in some cases the boundary conditions on both sides of the film are significantly different and this asymmetry should also be taken into account. The influence of the confining potential U_{conf} on the electrical conductivity of single semiconducting films was already studied by Gottinger *et al.*,[24] who showed that the weaker confining potential the smaller surface contribution to the resistivity.

Recently, a related formalism was developed for electronic transport in trilayers, and applied to magnetic sandwich structures.[25,26] We adopted this formalism to a description of electronic transport in single metallic films, which allows us to include all the factors mentioned above, i.e., different boundary conditions on both film surfaces (different confining potentials and different surface roughness) and scattering of electrons by bulk structural defects. The formalism allows us to calculate the electrical conductivity for metallic and semiconducting films with an arbitrary number of occupied minibands. It can be used in the case of a constant chemical potential μ, as well as in the case when the number of particles is conserved. Some numerical results obtained in the metallic limit (large N) are presented below.

The dependence of the electrical conductivity on the correlation length ξ is shown in Fig. 5 for a finite confining potential, constant chemical potential, and infinite bulk electron mean free path λ. The dependence is similar to that shown in Fig. 3, i.e., for each value of H the conductivity increases with increasing ξ. The dependence of the film resistivity on the fractality parameter H is shown explicitly in Fig. 6 for several values of the bulk electron mean free paths, but for a constant correlation length ξ. It is evident that bulk scattering processes reduce the surface fractality effects in the electrical conductivity. Finally, variation of the electrical resistivity with the film thickness d is shown in Fig. 7 for several values of the fractality parameter H. For all curves shown in Fig. 7, the conductivity increases on average with increasing d, with saw-shaped oscillations superimposed. The oscillation period is equal to half of the corresponding Fermi wavelength. The saw-shaped oscillations are characteristic of the model, and were also found in other descriptions.[12,25] The amplitude of the oscillations as well as their shape significantly depend on the factor H. For large H the oscillations are more pronounced than for small values of H.

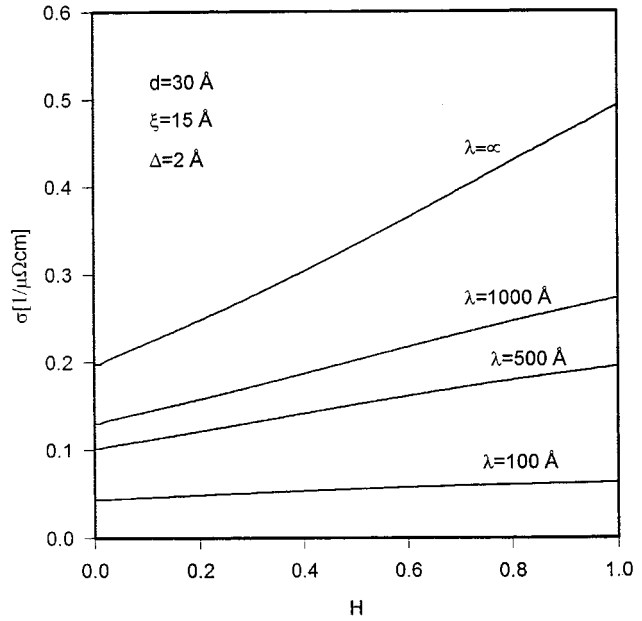

FIG. 6. Conductivity σ vs roughness exponent H for $U_{\text{conf}}=8.5$ eV, $\mu=3.5$ eV, and $a_0=0.3$ nm. The other parameters are as indicated.

VIII. CONCLUSIONS

In conclusion, we combined known information of the surface/interface roughness effect on the conductivity of thin

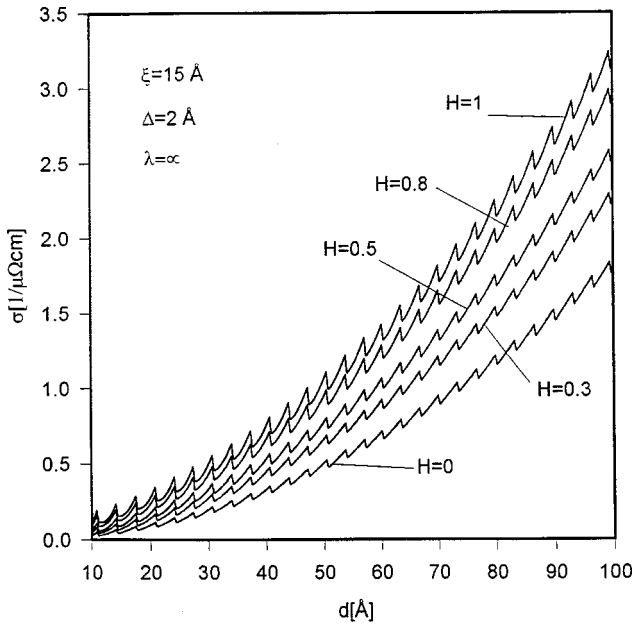

FIG. 7. Conductivity σ vs film thickness d for $U_{\text{conf}}=8.5$ eV, $\mu=3.5$ eV, and $a_0=0.3$ nm. The other parameters are as indicated.

films (metallic films, and semiconducting quantum wells), with those of analytic correlation models for self-affine fractal topography in order to examine fractality effects in the film conductivity. Such an examination was performed over a wide range of surface morphologies, from logarithmic ($H=0$) to power-law roughness (self-affine, $0<H<1$).

We limited our calculations to semiconducting quantum wells ($N=1$) and metallic ($N\gg 1$) films. Among the three surface/interface roughness parameters (Δ, ξ, and H) the main interplay of the roughness effect occurs for the last two, namely, H and ξ. The parameter Δ has a trivial effect on the conductivity since it appears in the form of a multiplication factor ($\sigma\sim\Delta^{-2}$). The roughness exponent H has a strong impact on the conductivity mainly for relatively large correlation lengths. Therefore, the degree of surface/interface irregularity must be taken carefully into account before deducing roughness correlation lengths from conductivity measurements. However, one has to bear in mind that the calculations presented above are based on the Born approximation. Consequently, some deviations from the exact conductivity may occur for large roughness amplitudes or for long correlation lengths.

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